# Ultra-high fidelity qubits for quantum computing

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We analyze a system of fermionic $^6$Li atoms in an optical trap, and show that an atom "on demand" can be prepared with ultra-high fidelity, exceeding 0.99998. This process can be scaled to many sites in parallel, providing a realistic method to initialize N qubits at ultra-high fidelity for quantum computing. We also show how efficient quantum gate operation can be implemented in this system, and how spatially resolved single-atom detection can be performed.

The potential impact of quantum computing has stimulated a worldwide effort to develop the necessary experimental and theoretical resources [1, 2]. The most challenging aspect of quantum computing is the requirement for ultra-high fidelity in each step. The necessary starting point is initialization of a scalable number of qubits at ultra-high fidelity. In this Letter, we consider a system of fermionic atoms and show that an atom "on demand" can be prepared in the ground state of a trap with fidelity exceeding 0.99998, providing a realistic solution to the initialization problem in quantum computing. We discuss how that process can be scaled to many sites in parallel, enabling pairwise entanglement operations. Finally we show how spatially resolved detection of each state can be implemented.

We first address the question of how to trap one atom "on demand" in the ground state of a trap. Note that such a process should be scalable up to many optical traps in parallel. A single atom "on demand" in the ground state has not yet been demonstrated experimentally. However, progress has been made for bosonic atoms using the method of laser culling [3, 4, 5]. One of the key questions is that of fidelity of the number state, and in that regard bosons are not ideal because they rely on strong interactions to maintain a relatively large excitation gap, and to suppress low-frequency excitations during the culling process. This leads us to propose instead fermionic atoms where a precise number is rigorously enforced by the Pauli exclusion principle. More specifically, we propose to use $^6$Li as the atom of choice. This atom has the advantage that the interaction strength and sign (attractive or repulsive) can be tuned with an external magnetic field. Two magnetic sublevels of one hyperfine ground state, $\left|F = \frac{1}{2}, m_F = \frac{1}{2}\right\rangle$ and $\left|F = \frac{1}{2}, m_F = -\frac{1}{2}\right\rangle$ are used to define a qubit. We denote these states as $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. These states both become high-field seekers at large magnetic field with a well-defined frequency splitting that is nearly field-independent, hence insensitive to magnetic noise.

The starting point of the "on demand" single atom preparation is laser-cooled $^6$Li atoms that are optically trapped in the two spin states [6, 7]. The atoms can be cooled by evaporation at a magnetic field around 300 Gauss, where the scattering length $a_s \approx -300a_0$ ($a_0$ is the Bohr radius). $a_s$ is large enough for efficient evaporation of the spin mixture, and is also at a minimum as a function of magnetic field, greatly reducing the effects of magnetic noise. After evaporative cooling, a weakly interacting degenerate Fermi gas forms at temperature $T \ll T_F$, where $T_F$ is the Fermi temperature. The single atom preparation process can be split into three steps:

**Step I** The magnetic field is tuned to near $\sim 0$ Gauss from the initial field of 300 Gauss, resulting in a non-interacting degenerate Fermi gas (DFG). In this state, a spin pair fills each level, up to approximately the Fermi level.

**Step II** Atom pairs are ejected by laser culling. This is accomplished by adiabatic lowering of the optical potential. This prepares a single pair in the ground state.

**Step III** The well is adiabatically split into two parts that are spatially separated. In the presence of a magnetic field bias this prepares one spin state on the left and the other on the right. Each atom can then serve as the initial state for a qubit.

With this method, an array of $N$ micro-traps would prepare $2N$ qubits. We now show in detail how ultra-high fidelity is enforced at each step.

**Step I** In the presence of a scattering length $a_s \approx -300a_0$ between the $|\uparrow\rangle$ and $|\downarrow\rangle$ states, the Fermi gas is weakly interacting. At $T = 0$, the Fermi gas may form a BCS state. The pairing gap for such a state can be estimated through $\Delta \approx 0.5E_F \exp\left(\pi/2k_F a\right)$ [8]. For a degenerate $^6$Li gas with $k_F^{-1} \sim 1000a_0$, the pairing gap $\Delta \approx 0.002E_F$. With such a small $\Delta$, the occupation probability of the lowest energy state (*e.g.* the $\mathbf{k} = \mathbf{0}$ state for a uniform gas) $n_{\mathbf{k=0}} = (1 - \eta_{\mathbf{k}}/\epsilon_{\mathbf{k}})/2 \approx 1 - 4 \times 10^{-6}$, where $\eta_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - E_F$, $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/2m$, $\epsilon_{\mathbf{k}} = \left(\Delta^2 + \eta_{\mathbf{k}}^2\right)^{1/2}$ is the quasi-particle excitation energy, and we take the chemical potential $\mu \approx E_F$ for the BCS state. In addition, for such a small pairing gap, finite temperature effects dominate, and there may even be no BCS pairing. However, the finite temperature does not affect the ground state occupation probability. Consider a temperature $T = 0.05T_F$, for
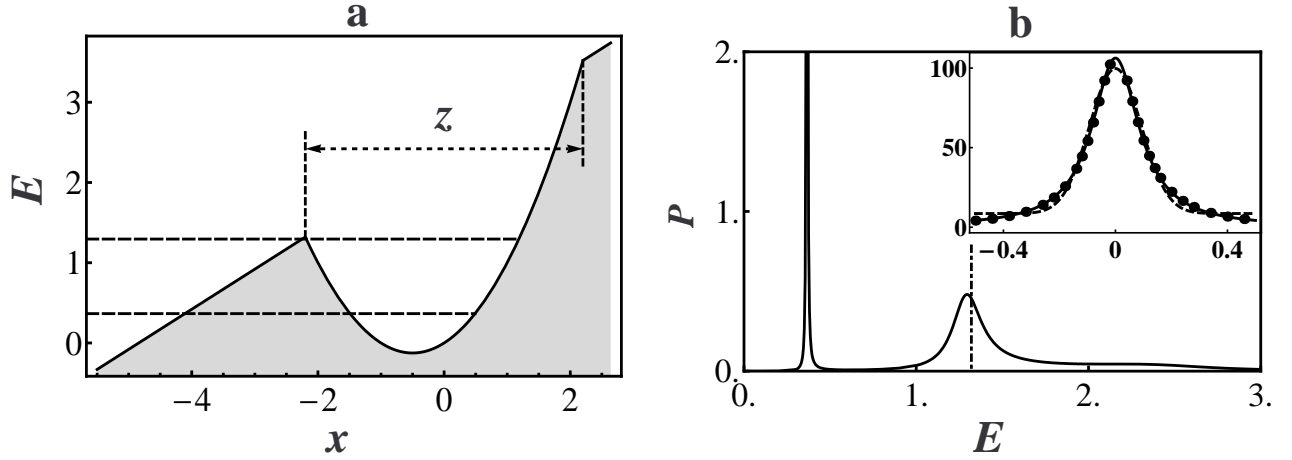
Figure 1: The simulation model for laser culling in a 1D optical trap. We take $x_0 \equiv \sqrt{\hbar/m\omega}$ as the unit of length ($m$ is the mass of the $^6$Li atom), $\hbar\omega$ as the unit of energy, and $\hbar\omega/x_0$ as the unit of force. **a** Truncated harmonic trap with magnetic gradient. The trapping potential for one state is shown. Parameters used to specify the trap: trap size, $z$, is the length of the parabolic portion in the potential profile; force, $f$ is the slope of the linear portion in the potential profile. Dashed lines denote the levels of the ground and first-excited states. **b** Plot of $P(E)$ as a measure of density of states of the quasi-bound states. Trap size $z = 4.4$, force $f = 0.5$. The vertical line (dotdashed) denotes the barrier height of the trap. Inset: Zoomed-in view of the resonance peak of the ground quasi-bound state (dots) as shown in the main figure and Lorentzian (solid) and Gaussian (dashed) regressions. Horizontal axis is in units of $\gamma/2$, where $\gamma$ is the FWHM of the resonance peak.

which the ground state occupation probability is approximately $1/\left[\exp\left(-E_F/k_BT\right)+1\right] = 1 - 4 \times 10^{-5}$. Therefore, a fast sweep of the magnetic field (i.e., the scattering length) to the non-interacting region does not affect the ground state occupation probability or the fidelity of the single atom preparation.

**Step II** A non-interacting DFG in a deep optical trap serves as the starting point for the laser culling process. We assume that the trapping frequencies in the two transverse directions are significantly higher than along the axis, and only the ground transverse state can be supported. We therefore limit our analysis to one spatial dimension. The trap wall is reduced to a level slightly below the ionization threshold of the first-excited state of the optical dipole trap. The trap reduction rate is chosen to fulfill the adiabaticity requirement. To that end, we maintain a constant trapping frequency, $\omega$, throughout the laser culling process, which can be accomplished by dynamically varying the focus of the beam [9]. (In practice, this step may not be necessary, but it greatly simplifies the calculation.) According to the Wentzel-Kramers-Brillouin (WKB) method, atoms with energy much lower than the trap depth are completely unaffected by the change in the depth of the trap. The adiabaticity condition is fulfilled as long as the WKB approximation is valid, which holds until the trap depth is around $3\hbar\omega/2$, where $\hbar \equiv h/2\pi$ and $h$ is Planck's constant. Near and beyond this point, the trap reduction rate must be slowed down to maintain adiabaticity.

A constant force (or tilt), $f$, is also needed to sweep the atoms away from the micro-traps as soon as they are ionized, which is generated by applying a magnetic field gradient. For simplicity, we assume the force has a positive sign for state $|\uparrow\rangle$. In our simulation, we approximate the optical trap with a truncated harmonic potential (see Fig.1**a**) which is specified by the *trap size*, $z$. After reaching a minimum trap size $z_m$, the trap is held for a certain time to allow ionized atoms to escape, while keeping the ground-state atom pair with high probability. The trap depth, magnetic force, and holding time are adjusted to optimize fidelity. Finally the trap wall (and size) is adiabatically raised to a higher level to preserve the resultant Fock state.

Our simulation method is described below. We assume that the ground state fidelity is unchanged until the ionization energy of the first excited state is approached. Because of the tilt, the trap has no stationary bound state, only quasi-bound states, which, as $z \to \infty$, become the bound states. The lifetimes of the quasi-bound states determine the rate of the change of trap occupation probability. The optimized final trap depth, tilt, and holding time is calculated.

Suppose a stream of incoming atoms is incident from $x = -\infty$, with energy $E$, scattered by the trap potential. Let $\psi_E(x)$ be the wavefunction of the stationary state of the incoming atoms, which is assumed to have unit amplitude at $x = -\infty$. We assume the trap is located at $[-z/2, z/2]$. Outside the trap ($x < -z/2$), $\psi_E(x)$ is a superposition of Airy functions Ai$(x)$ and Bi$(x)$ with necessary superposition amplitudes and phases; inside the trap,

$$\psi_E(x) = a(E)e^{-x^2/2}H_\nu(x), \qquad (1)$$

where $H_\nu(x)$ is the Hermite function of degree $\nu$, $a(E)$

is the amplitude. We require $\psi_E(x)$ be continuous and differentiable for all $x$, by which $a(E)$ is obtained. Of special interest to us are those states that have significant amplitude in the trap area, because they correspond to the quasi-bound states of the trap. We define $P(E) \equiv |a(E)|^2$. For simplicity, we can take $P(E)$ as a measure of the density-of-states of the trap. We plot $P(E)$ in Fig. 1b. Note that in the limit of zero magnetic force, the peaks at $E \approx 0.366$ and $1.29$ correspond to the ground and first-excited states of the truncated harmonic trap, respectively.

$P(E)$ describes not only the ionization thresholds, but also the dynamical properties of the quasi-bound states. To see that, we study the evolution of a wavefunction $\phi(x, t)$. Imagine that at time $t = 0$, we have

$$\phi(x, 0) = \begin{cases} c\,\psi_{E_0}(x), & -z/2 < x < z/2; \\ 0, & \text{otherwise,} \end{cases} \quad (2)$$

where $E_0$ is one of the resonance energies, $c$ is a normalization factor such that $\int_{-\infty}^{\infty} |\phi(x,0)|^2 dx = 1$ and there is no other atom source. Subsequently, the atom will start to tunnel out of the trap. The probability, $R_{E_0}(t)$, for an atom to remain in the trap is given by $\int_{-z/2}^{z/2} dx\, |\phi(x,t)|^2$. To evaluate $R_{E_0}(t)$, we expand $\phi(x,t)$ in terms of the wavefunctions of the stationary states, $\psi_E(x)$. Note that in the vicinity of a resonance peak at $E = E_0$, one can write the wavefunction $\psi_E(x) \approx C(E)a(E)\psi_{E_0}(x)$, where $C(E)$ is a slowly varying quantity. Also

$$\int_{-z/2}^{z/2} dx\, \psi_E^*(x)\psi_{E_0}(x) \approx \int_{-\infty}^{\infty} dx\, \psi_E^*(x)\psi_{E_0}(x) \quad (3)$$

for $E \neq E_0$, due to the oscillatory nature of Airy functions. We find

$$R_{E_0}(t) \approx |C(E_0)|^2 \left| \int_{E_0 - \epsilon/2}^{E_0 + \epsilon/2} P(E)e^{iEt} dE \right|^2, \quad (4)$$

where $\epsilon$ is the range of integration. In the vicinity of a resonance peak, the function $P(E)$ is essentially Lorentzian (see inset of Fig. 1b), and we finally obtain

$$R_{E_0}(t) \approx e^{-\gamma_{E_0} t}, \quad (5)$$

where $\gamma_{E_0}$ is the full width at half maximum (FWHM) of the resonance peak at $E = E_0$. The lifetime of the quasi-bound state at $E = E_0$ is $\tau_{E_0} = \gamma_{E_0}^{-1}$. Eq.(5) is used to determine an optimized combination of minimum trap depth, magnetic force, and holding time for the best fidelity. It is also worth noting that ultimately the *difference* in the lifetimes between the ground and the first excited quasi-bound states determines the fidelity of producing a pair of atoms in the ground state of the trap.

Taking into account all the steps in laser culling, we show the fidelity of preparing a single pair of atoms in ground state of a micro-trap in Fig 2. Choosing culling
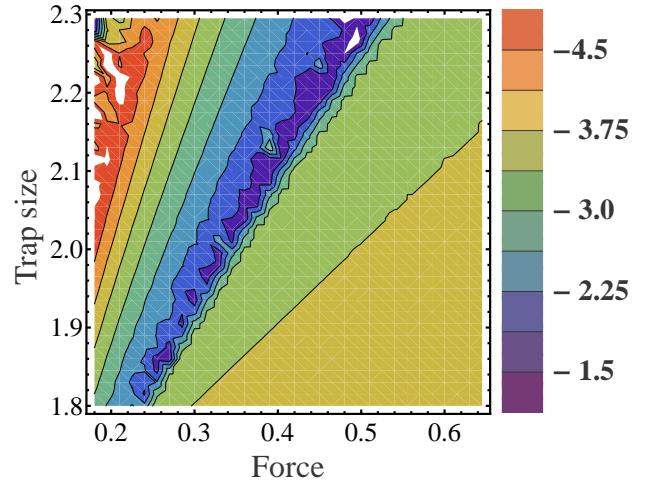


Figure 2: Ground state fidelity after laser culling. A varying holding time is allowed to ensure that the residual probability for atoms in excited quasi-bound states is no larger than $10^{-5}$. Shown in the panel is the base-10 logarithm of the ground state fidelity loss. Red (blue) color represents high (low) fidelity. The white areas are out-of-range clippings: near the left-hand side, the white areas should be redder than its surrounding color; near center-top, the white area should be bluer than its surrounding color.

parameters near the upper-left corner of the figure results in ultra-high fidelity. For a set of realistic parameters: trapping frequency $\omega = 2\pi \times 1$ kHz, magnetic field gradient 0.66 Gauss/cm, and truncated trap size 8.8 $\mu$m, the ground-state to first-excited state lifetime ratio is $7.53 \times 10^5$. With a holding time of 218 ms, we get a residual probability of $10^{-5}$ for the excited-state and a ground state occupation probability larger than 0.99998.

**Step III** Finally, the pair of atoms are split and trapped in the ground state of two adjacent micro-traps. In order to achieve deterministic splitting, where one spin state is driven to the left and the other to the right, we impose a magnetic field gradient (providing a force $f$) while we adiabatically split the optical tweezer (that holds the pair) into two beams [10]. With an appropriate magnetic field gradient and a separating barrier, this step can be realized at ultra-high fidelity. Since $|\downarrow\rangle$ is a low-field-seeker and $|\uparrow\rangle$ is a high-field-seeker at low magnetic field, each atom is displaced to a different location as soon as the trap is split.

We adopt a simpler potential than that of a realistic optical tweezer. The trap is composed of two spliced sections of parabolic trap with identical trapping frequency $\omega$, each of which has an energy minimum, located at $\pm d/2$, respectively, where $d$ is the separation distance. We numerically calculate the eigen-energy levels and wavefunctions of such a double-well structure in the parameter space of $f$ and $d$. One needs to choose a path in the parameter space such that a sufficient gap between the ground and first-excited states is maintained

throughout the splitting process in order to suppress transitions from the ground state. With a trapping frequency $\omega = 2\pi \times 1$ kHz, a magnetic field gradient of 0.66 Gauss/cm and a separation displacement $d = 6.25$ $\mu$m, we find 0.99998 splitting fidelity.

So far, we have shown that two initialized fiducial states can be prepared at ultra-high fidelity. How can one scale this process to multiple sites, and make the "switchyard" of multiplexed beams to perform the required complex operations? The scalability of this system can be achieved using scalable microelectromechanical systems (MEMS) technology [11]. Using this technology, an array of beams can be directed to each site where individual atoms can be trapped. An alternative approach was developed in ref. [12]. By steering the beams, one can transport individual atoms and bring them into pairwise interaction with arbitrary control. An array of micro-traps would most easily be accomplished with red-detuned beams that create attractive potentials along the axis. This technique also enables the creation of a two-dimensional optical trap array, and entanglement of any pair using the qubit transfer technique of ref. [10]. This could extend the linear case where only nearest-neighbor operations are possible.

We now consider single-qubit gates and two-qubit gates in this system. The implementation of a single-qubit gate requires the capability to address each atom individually. This can be accomplished with stimulated Raman transitions, as is currently employed with trapped ions [13, 14] and with neutral atoms [15]. The realization of a two-qubit gate can be based on collisions between bosonic atoms [16]. This scheme was realized experimentally with atoms in an optical lattice [17]. Fermionic atoms in the same internal state cannot collide due to the Pauli exclusion principle. However, atoms in different states can have a large collisional shift, which can be used to engineer two-qubit SWAP (or $\sqrt{\text{SWAP}}$) gates, as proposed in ref. [18]. The scattering length can be made very large by tuning closer to the Feshbach resonance. For a set of parameters $\omega = 2\pi \times 1$ kHz and $a_s \sim 330a_0$, a high fidelity $\sqrt{\text{SWAP}}$ gate can be implemented in a time period of about 40 ms. We envision that with an array of many qubits, a sequence of $\sqrt{\text{SWAP}}$ operations can build scalable entanglement in this system. This two-qubit operation, together with single-qubit rotations, provides a set of universal quantum gates.

The detection of each qubit state at the end of a quantum computation can be accomplished by spatially-resolved fluorescent imaging [19, 20]. This stage must also resolve the spin of each location. This can be accomplished with the same method that was used to separate the spin pair, followed by fluorescent imaging.

One important consideration is the limitation on fidelity set by decoherence. One fundamental source is light scattering by the optical tweezers. The scattering rate is proportional to the third power of the frequency.

This was the motivation for using a $CO_2$ laser for optical trapping [7]. In our case, such a laser can be used for trapping in two transverse directions where the trap depth must be higher. This would confine the atoms along a line. However, the optical tweezers that implement logic gates must be at a shorter wavelength in order to have sufficient spatial resolution. The trap depth in this direction need only be enough to contain the ground state, so we estimate that light scattering will not limit the quoted fidelity. Other sources of decoherence are laser intensity noise and pointing noise. The fundamental limit in this case is shot noise, and should also not limit the predicted fidelity.

In conclusion, we find that fermionic atoms can be used to realize ultra-high fidelity for quantum computing. Future work will analyze the optimum strategies for pairwise entanglement in this system.

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